COMPUTATION OF LIGHT SCATTERED INTO A DETECTOR

Egon Marx
National Institute of Standards and Technology
Gaithersburg, MD 20899

INTRODUCTION

To compare the measured bidirectional reflectance distribution function (BRDF) of a rough surface to the results of a computation, we have to take into account the aperture of the detector and, more generally, the properties of the measuring instrument. We either integrate the computed angular distribution of the scattered intensity over the solid angle subtended by the detector or convolve the angular distribution with the measured instrument signature. Effects due to the detector are most important when the specular beam is large compared to the diffuse scattering intensity and is included in the light gathered by the detector. We also have to perform such an integration to average over the variations of the scattered intensity due to speckle. We first consider a one-dimensionally rough surface and then we extend the methods to the more general isotropic, rough, flat surface. The angular distribution of the scattered light intensity is proportional to the BRDF multiplied by the cosine of the scattering angle. We usually normalize the computed values of the scattered light intensity by matching the peak intensity in the specular direction to the measured value. The absolute intensity of the scattered light is difficult to compute, especially when the surface is not perfectly conducting. Windowing effects have to be included in the computation of the field amplitudes in the Kirchhoff approximation.

ONE-DIMENSIONALLY ROUGH SURFACES

We assume that the surface and the incident light beam extend to infinity in the y-direction and that the scatterer is invariant under displacements in that direction. The angular distribution of the scattered light as a function of the scattering angle, $I(\theta)$, can be computed from a simulated or measured surface topography map using, for instance, the Kirchhoff approximation applied to the scalar wave equation [1]. The light collected by a detector that subtends an angle $2\theta_d$ is then proportional to

$$I_d(\theta) = \int_{\theta-\theta_d}^{\theta+\theta_d} I(\theta')d\theta' \approx \Delta\theta \sum_{i=-n}^{n} I(\theta + i\Delta\theta), \qquad (1)$$

where $n \approx \theta_d/\Delta\theta - ½$. We are approximating $I(\theta)$ by a constant over each interval $\Delta\theta$, which may not be a good approximation where this function varies rapidly, mainly near the specular direction when a specular beam is significant. To improve the accuracy, we subdivide some of the intervals and recompute the integral, continuing until the change in the integral is below a given threshold.

Actual detectors are circular instead of extending to infinity in the y-direction. In a one-dimensional scattering problem, the direction of propagation of the scattered light lies in the xz-plane, which is not exactly true for the measured intensities. We have to measure the light scattered slightly off that plane and add the contributions, as discussed in [2], to improve the agreement between measured and computed intensities.

ISOTROPIC RANDOM ROUGH FLAT SURFACES

Similar considerations apply to the scattering by a flat surface that is rough in two dimensions. The electromagnetic field amplitude of the light scattered by a surface $z = \zeta(x,y)$ in the Kirchhoff approximation using a windowing function, $W(x,y)$, is

$$\psi(\theta,\varphi) = [F_3(\theta,\varphi)/A]\int_\Sigma W(x,y)\exp[i\vec{v}(\theta,\varphi)\cdot\vec{x}(x,y)]\,dxdy\,, \tag{2}$$

where Σ is the illuminated surface, A is the corresponding area, and, if θ_i is the angle of incidence,

$$F_3(\theta,\varphi) = \frac{1 + \cos\theta_i\cos\theta + \sin\theta_i\sin\theta\cos\varphi}{\cos\theta_i(\cos\theta_i + \cos\theta)}\,, \tag{3}$$

$$\vec{v}\cdot\vec{x} = -k[(\sin\theta_i + \sin\theta\cos\varphi)x + (\sin\theta\sin\varphi)y + (\cos\theta_i + \cos\theta)\zeta(x,y)]\,. \tag{4}$$

The scattered intensity is a function of the polar and azimuthal angles, and the light scattered into a detector defined by a solid angle Ω_d is given by

$$I_d(\theta,\varphi) = \int_{\Omega_d} I(\theta',\varphi')\,d\Omega'\,, \tag{5}$$

which generalizes (1). A rotation in the coordinates that brings the (θ,φ) direction to the z-axis is helpful in determining the angles where the intensity has to be computed to cover the solid angle of the detector. If the measurements are restricted to the plane defined by $\varphi = 0°$ and $\varphi = 180°$, we can assume that the specular peak is symmetric about the specular direction to simplify the integration for the light scattered in the specular direction and obtain

$$I_d(\theta_{sp}) \approx 2\pi\int_{\theta_{sp}-\theta_d}^{\theta_{sp}+\theta_d} I(\theta')\,d\theta'\,. \tag{6}$$

Such an approximation is more difficult to justify for an arbitrary position of the detector. The sine factor in the element of solid angle is approximately equal to 1.

CONVOLUTION WITH THE INSTRUMENT SIGNATURE

The instrument signature is obtained by measuring the light intensity detected in the absence of a sample or with a sample that is a nominally perfect mirror for different angles of incidence. The illuminated surface is determined by the size of the incident beam, which is subsequently focused on the detector. The signature also reflects the aperture of the detector. When the detector is placed in the direction of the

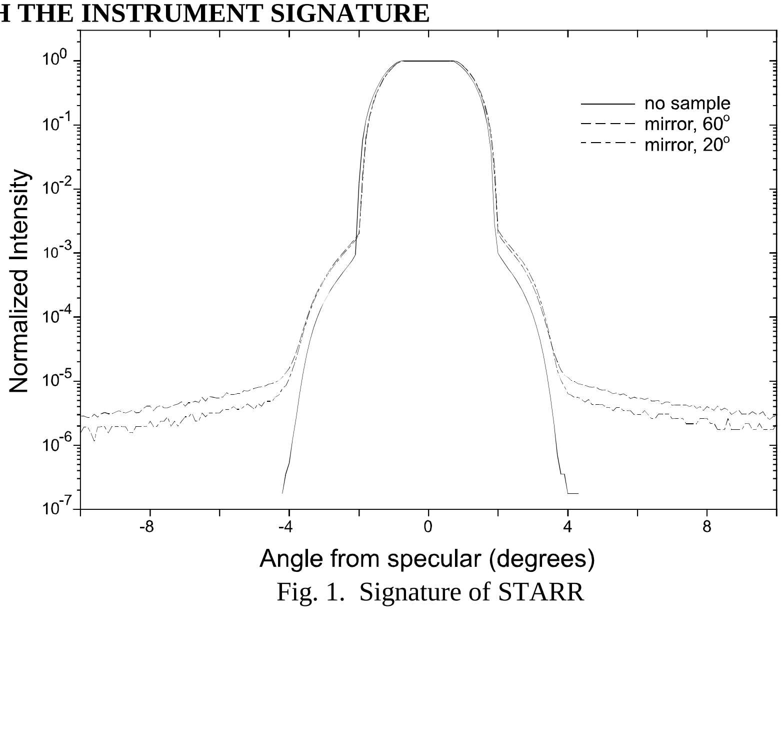

Fig. 1. Signature of STARR

incident (or specular) beam, essentially all the light is collected. As the detector is displaced, the measured intensity remains constant until the edge of the detector cuts off part of the beam. Then it decreases gradually until no part of the beam is collected by the detector. The intensity is reduced to approximately one half of the maximum when the center of the beam reaches the edge of the detector. Light scattered by other surfaces inside the instrument also affects the instrument signature in the form of stray light. In Fig. 1 we show the instrument signature for the NIST spectral tri-function automated reference reflectometer (STARR) [3] measured with a mirror in place for a direction of incidence of 20° and 60°, normalized to 1 in the specular direction, compared to the signature taken in the absence of a sample. We can represent this signature or response function by $I_r(\theta,\varphi;\theta',\varphi')$, where θ and φ define the position of the detector and θ' and φ' define the direction of the incident light in the absence of a target, or the specular direction if the sample is a perfect mirror. Then the measured intensity can be expressed as an integral of the computed intensity scaled by the instrument signature, that is,

$$\bar{I}(\theta,\varphi) = \int_\Omega I(\theta',\varphi')I_{4r}(\theta,\varphi;\theta',\varphi')d\Omega' , \tag{7}$$

where the subindex 4 refers to the number of arguments and Ω is the solid angle over which the incident beam can be varied in the determination of the signature. We can assume that the signature is independent of the direction of incidence, that is, that only the relative positions of the detector and the beam matter, whence $I_{4r}(\theta,\varphi;\theta',\varphi') = I_{2r}(\theta - \theta',\varphi - \varphi')$. If we can only measure the instrument signature along a fixed plane, we obtain a response function $I_r(\theta)$. Then (7) reduces to

$$\bar{I}(\theta) = \int_{\theta_1}^{\theta_2} I(\theta')I_r(\theta - \theta')d\theta' , \quad -\tfrac{1}{2}\pi < \theta < \tfrac{1}{2}\pi . \tag{8}$$

Using the range $[-\tfrac{1}{2}\pi,\tfrac{1}{2}\pi]$ for the polar angle θ and a fixed azimuthal angle φ is equivalent to using the range $[0,\tfrac{1}{2}\pi]$ for θ and both φ and $\varphi + \pi$ for the azimuthal angle. The integration carried out according to (8) is usually called a convolution, although the range of integration is finite. If we assume that we have computed $I(\theta)$ and measured $I_r(\theta)$ for $-\tfrac{1}{2}\pi \le \theta \le \tfrac{1}{2}\pi$, the limits of integration are $\theta_1 = \max(-\tfrac{1}{2}\pi, -\tfrac{1}{2}\pi - \theta)$ and $\theta_2 = \min(\tfrac{1}{2}\pi, \tfrac{1}{2}\pi + \theta)$. In practice, measurements cannot be carried out very close to grazing angles. The most important effects of this integration are to flatten the top of the curve and to smooth the oscillations due to speckle. If the signature consists of a sharp peak and can be represented by a δ-function, we find from (8) that $\bar{I}(\theta) = I(\theta)$.

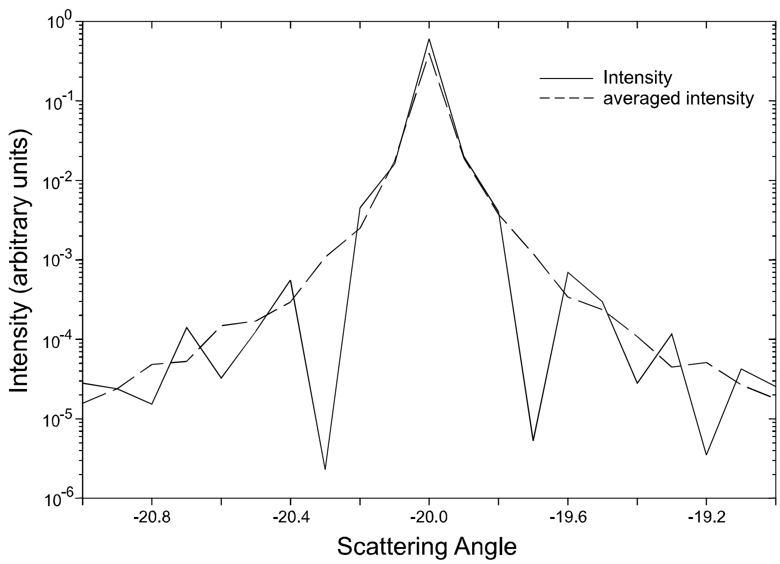

Fig. 2. Field intensities near the specular peak.

The assumption that the integrand remains constant in each interval $\Delta\theta$ in the numerical evaluation of the integral in (8) is a reasonable approximation, in spite of the variations due to the existence of speckle, except for detector positions near the specular value if the roughness is small enough to produce an identifiable specular beam. In this case we should subdivide those intervals to the side of the specular direction and average the computed values. One can check how much the value changes by subdividing the interval and calculating new simulated intensities to decide whether further subdivision is necessary. The main difference is obtained for the average value including the peak itself, as those in the neighborhood of the peak will be unchanged if the curve is nearly linear. The effects of the averaging for a very smooth surface (rms roughness of ~2.6 nm compared to the wavelength of light of 550 nm) can be seen in Fig. 2 for angles near the specular direction. The field intensities were computed using (2) for a measured surface topography map, and the averaging reduces the peak intensity by approximately one third. Results of other calculations can be found in [4].

WINDOWING FUNCTIONS

We have to take into account a real or fictitious intensity profile of the beam in the calculation of the scattered amplitude using (2). A windowing function W(x,y) equal to 1 over the region of integration represents a square window, which corresponds to an incident field that has jump discontinuities at the edges and vanishes outside the illuminated area. As a consequence of these approximations the computed amplitude decreases slowly as a function of angle, essentially as a sinc function for smooth surfaces. We thus have to use a more realistic shape for the incident beam in the calculation. For isotropic rough surfaces we have used a windowing function that is the product of two Schwartz functions, which are infinitely differentiable and of compact support. This function was found to yield good results for sinusoidal surfaces that have cylindrical symmetry [5]. The discontinuities in the function of the first derivative of other windowing functions can cause problems similar to those of a square window.

CONCLUSIONS

To compare a computed BRDF or intensity distribution to a measured one we have to consider at least three issues beyond the computation of the intensity as a function of scattering angle: the convolution with the instrument signature, averaging over intervals to take into account the specular peak and speckle, and the inclusion of a windowing function in the Kirchhoff approximation. Integration over the detector aperture can replace the convolution with the instrument signature.

ACKNOWLEDGMENTS

I wish to thank NIST staff members T. V. Vorburger and T. A. Germer for helpful comments, R. G. Dixson for the surface topography map, and M. E. Nadal for supplying the instrument signatures.

REFERENCES

[1] P. Beckmann and A. Spizzichino, *The Scattering of Electromagnetic Waves from Rough Surfaces*. New York: Pergamon, 1963.

[2] E. Marx and T. V. Vorburger, "Direct and Inverse Problems for Light Scattered by Rough Surfaces," Appl. Opt. **29**, 3613-3626 (1990). Reprinted in *Optical Methods in Surface Metrology*, David J. Whitehouse, Ed., Vol. MS129, 257-270, SPIE Optical Engineering Press (1996).

[3] P. Yvonne Barnes, Edward A. Early, and Albert C. Parr, *Spectral Reflectance*, NIST Special Publication 250-48 (1998).

[4] M. E. McKnight, E. Marx, M. E. Nadal, T. V. Vorburger, P. Y. Barnes, and M. Galler, "Measurement and Prediction of Light scattering by Coatings," submitted to *Appl. Opt.*

[5] E. Marx and T. V. Vorburger, "Windowing effects of light scattering by sinusoidal surfaces," in *Optical Scattering: Applications, Measurement, and Theory II*, J. C. Stover, Ed., Proceedings of the SPIE, Vol. 1995, 2-14 (1993).